Turbulent Combustion: Theory and Modelling
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Lecture-42
Turbulence – Chemistry Interaction (contd...)

So welcome back and we are doing the discussion the basics of the turbulent reacting system what you need and what are the governing equations and then we will continue the discussion.

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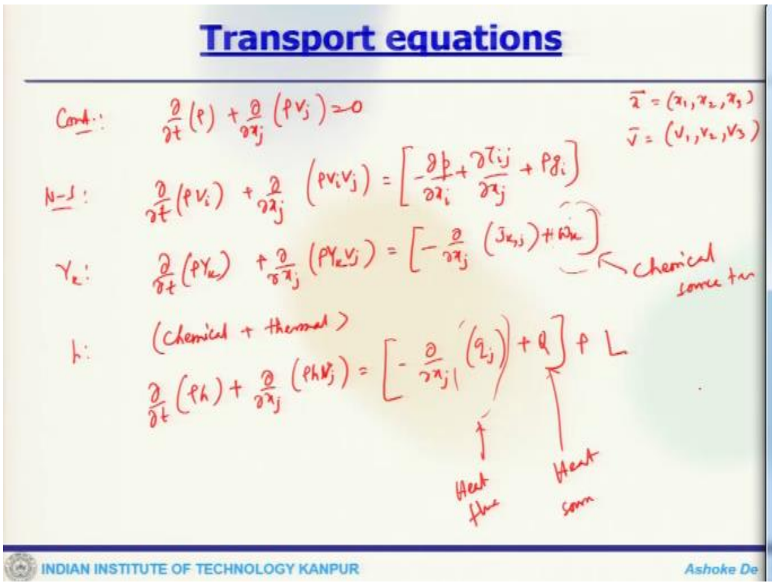

Transport equations

Cont.: $\frac{\partial}{\partial t}(\rho) + \frac{\partial}{\partial x_j}(\rho v_j) = 0$

$\bar{x} = (x_1, x_2, x_3)$

$\bar{v} = (v_1, v_2, v_3)$

N-S: $\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j) = \left[-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i\right]$

Y_k: $\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k v_j) = \left[-\frac{\partial}{\partial x_j}(J_{k,j}) + \dot{\omega}_k\right]$ ← chemical source ter

h: (chemical + thermal)

$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho h v_j) = \left[-\frac{\partial}{\partial x_j}(q_j) + Q\right] \rho L$

Heat flux

Heat source

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So this is where we start looking at all the set of equations that one need like all these transport equations.

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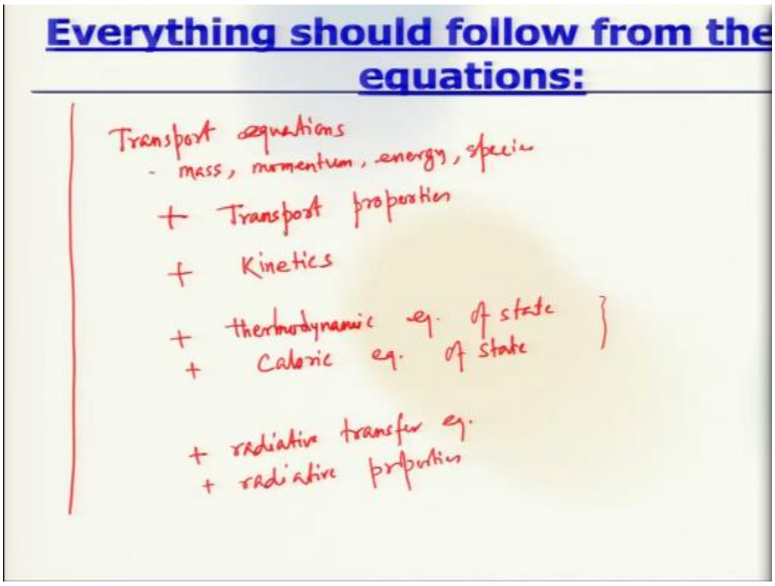

Everything should follow from the equations:

Transport equations
- mass, momentum, energy, species

\+ Transport properties

\+ Kinetics

\+ thermodynamic eq. of state

\+ Caloric eq. of state

\+ radiative transfer eq.

\+ radiative properties

Transport properties kinetics thermodynamic state and this that will get you continuity Navier Stokes species and this.

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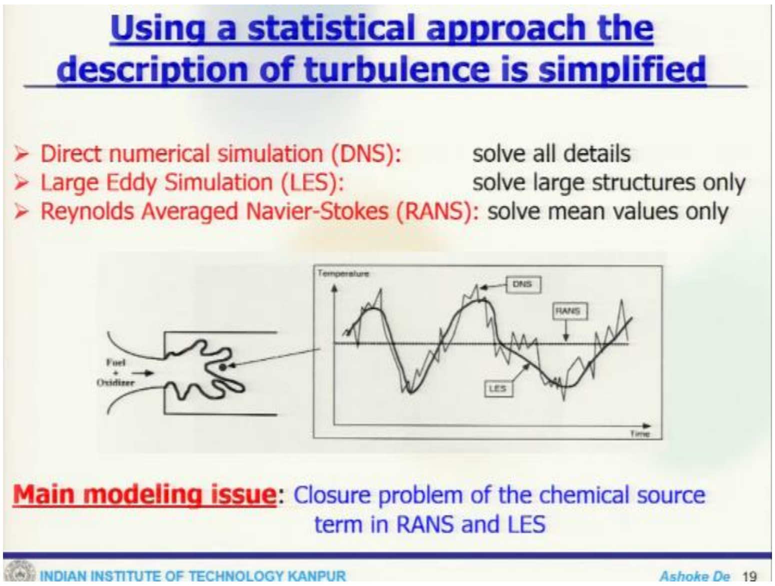

Using a statistical approach the description of turbulence is simplified

- Direct numerical simulation (DNS): solve all details
- Large Eddy Simulation (LES): solve large structures only
- Reynolds Averaged Navier-Stokes (RANS): solve mean values only

Main modeling issue: Closure problem of the chemical source term in RANS and LES

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Now there is a statistical approach description for the turbulence. This is already we have discussed in details because this is one of the issues in modeling when you look at the RANS which is very simple to use but only solve for the mean values whether LES solve for large scale structure, it models the small scale structure and when you look at DNS, it solves all details.

Now when you looked at the only turbulence system that time we did not need to bother about the reaction and other things which are quite critical under reacting system. So one of the issues which one more find is the closer problem of this chemical source term in both in RANS and LES, as long as we are doing DNS we resolve all the scale and we solve without any closure or any other assumption, but the when you come to LES or RANS, we need some closure thing.

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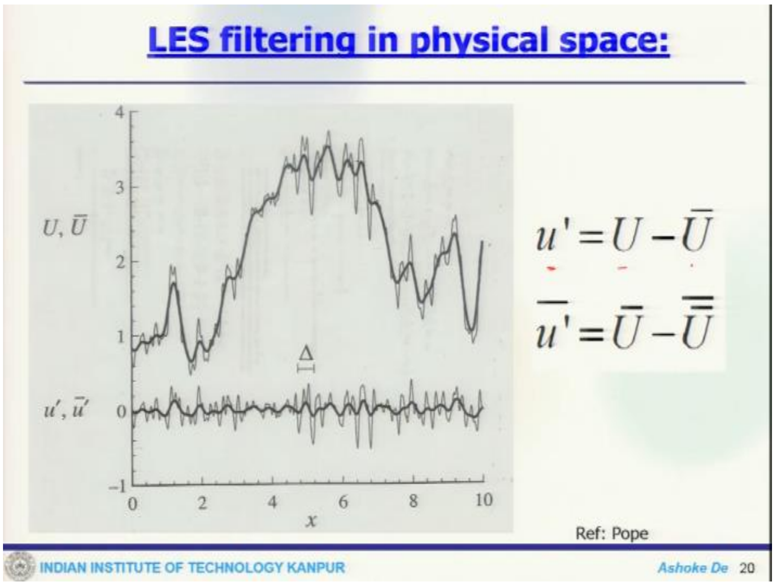

LES filtering in physical space:

$$u' = U - \bar{U}$$

$$\overline{u'} = \bar{U} - \bar{\bar{U}}$$

Ref: Pope

This is typically how a signal is represented because if you have a fluctuating component, which can be obtained from the instantaneous component minus the union value.

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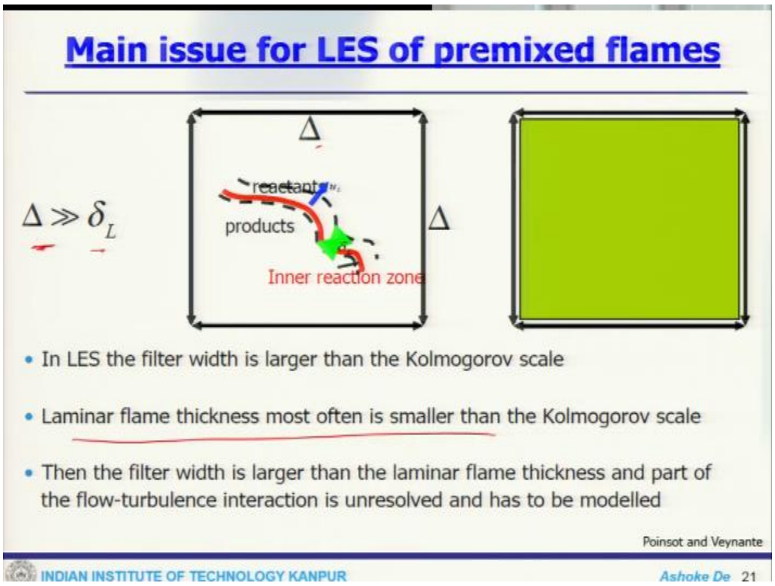

Main issue for LES of premixed flames

$\Delta \gg \delta_L$

- In LES the filter width is larger than the Kolmogorov scale
- Laminar flame thickness most often is smaller than the Kolmogorov scale
- Then the filter width is larger than the laminar flame thickness and part of the flow-turbulence interaction is unresolved and has to be modelled

Poinsot and Veynante

So when you go to some of the issues that will touch upon here then only going to the details of those particular discussion like premixed flame and something then we will see how that impact, now the one of the issue which will people find in LES of the premixed flame. So LES has a grid size like this or rather the filter size which is of order of delta. Now laminar flame thickness of the flame thickness of the premixed flame quite small or very small.

So what happens essentially the flame front sit inside and red cell. So which means the filter size of the grid size is quite larger than the thickness, so that allows I mean in different challenge to how to resolve this flame front. So this is what I mean this is quite small than the kolmogorov scale and the filter size is larger. So one need to be careful to handle that kind of situation whether the flame front may sit inside the grid cell.

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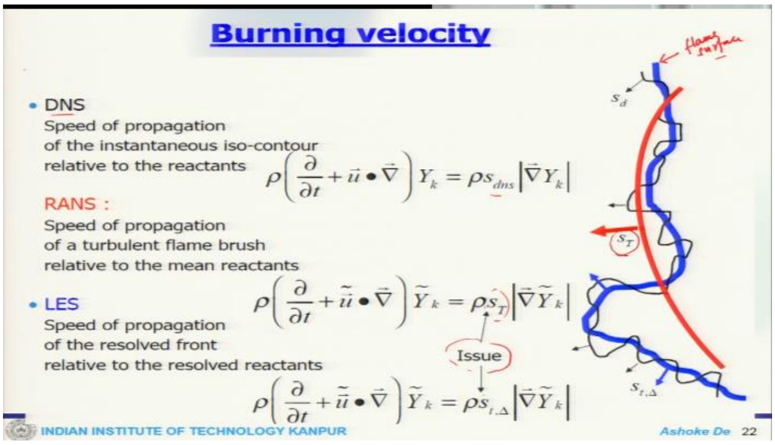

Burning velocity

- DNS
  Speed of propagation
  of the instantaneous iso-contour
  relative to the reactants

$$\rho\left(\frac{\partial}{\partial t}+\vec{u}\bullet\vec{\nabla}\right)Y_k=\rho s_{dns}\left|\vec{\nabla}Y_k\right|$$

RANS :
Speed of propagation
of a turbulent flame brush
relative to the mean reactants

$$\rho\left(\frac{\partial}{\partial t}+\tilde{\vec{u}}\bullet\vec{\nabla}\right)\tilde{Y}_k=\rho s_T\left|\vec{\nabla}\tilde{Y}_k\right|$$

- LES
  Speed of propagation
  of the resolved front
  relative to the resolved reactants

$$\rho\left(\frac{\partial}{\partial t}+\tilde{\vec{u}}\bullet\vec{\nabla}\right)\tilde{Y}_k=\rho s_{t,\Delta}\left|\vec{\nabla}\tilde{Y}_k\right|$$

Issue

Then another thing what will come is the flame front? This is our flame front or wrinkled flame front, this is the flame surface, so the burning velocity. So as long as we are dealing with the laminar burning will laminar flame, the only thing that we are concerned about the laminar speed but when you talk about the turbulent system, then there is a burning velocity you get in component which is known as turbulent flame speed. So for DNS the speed of propagation of the instantaneous iso contour, which is relative to the reactants?

So that is what the speed of the frame front. RANS the speed of propagation of the flame brush relative to the mean reactant. This is what you get in the laminar that is the turbulent burning velocity and LES also it is to the resolved. Now in RANS and LES this is an issue how we get the closure for the turbulent flame speed that requires some calculation.

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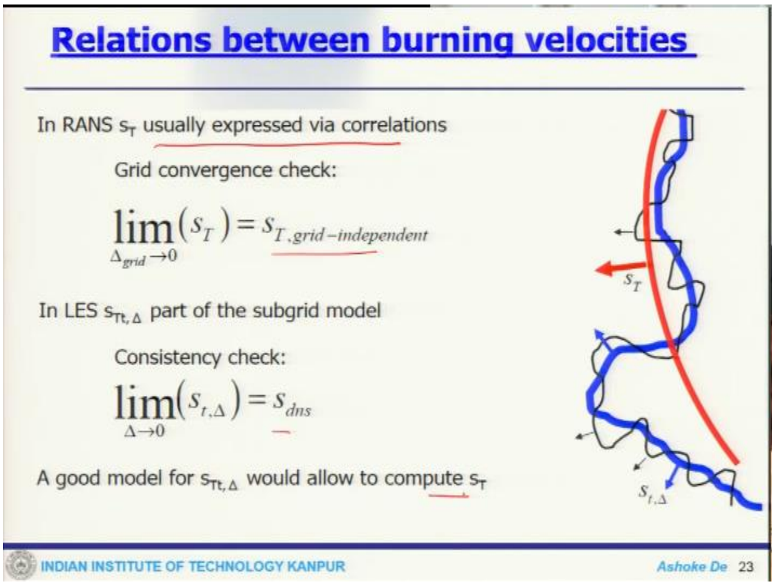

Relations between burning velocities

In RANS s_T usually expressed via correlations

Grid convergence check:

$$\lim_{\Delta_{grid}\to 0}(s_T)=s_{T,grid-independent}$$

In LES $s_{Tt,\Delta}$ part of the subgrid model

Consistency check:

$$\lim_{\Delta\to 0}(s_{t,\Delta})=s_{dns}$$

A good model for $s_{Tt,\Delta}$ would allow to compute s_T

Now typically in the RANS, it is usually expressed via some correlations. Now, if you grid tends to 0 then this becomes grid independent and also for LES part of the sub grid model. This should be approaching towards the flame speed that you get in the DNS, so but in good model should allow to compute the turbulent flame speed.

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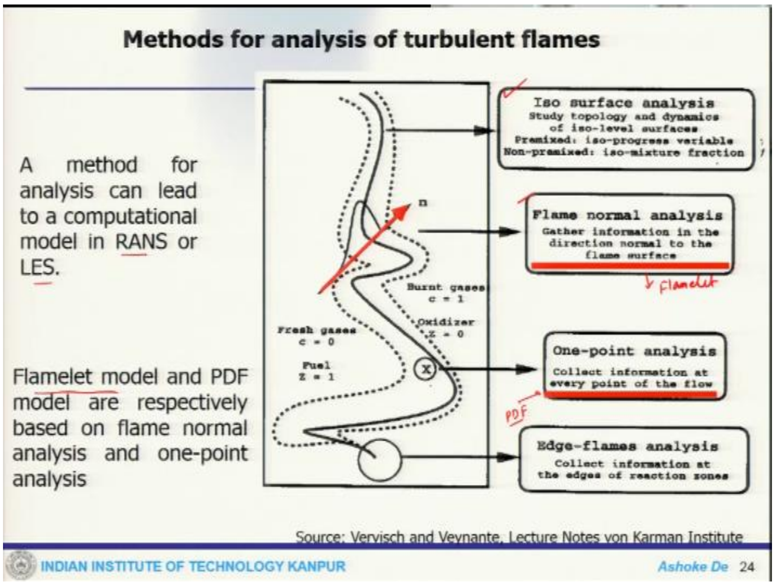

Methods for analysis of turbulent flames

A method for analysis can lead to a computational model in RANS or LES.

Flamelet model and PDF model are respectively based on flame normal analysis and one-point analysis

Iso surface analysis
Study topology and dynamics of iso-level surfaces
Premixed: iso-progress variable
Non-premixed: iso-mixture fraction

Flame normal analysis
Gather information in the direction normal to the flame surface

One-point analysis
Collect information at every point of the flow

Edge-flames analysis
Collect information at the edges of reaction zones

Source: Vervisch and Veynante, Lecture Notes von Karman Institute

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So if we put these things that there are different methods for analysis of this turbulence flame, now method depending on the method also RANS or LES things would change, now one option is that this is a typically a flame front and this is the normal across the flame front. So one approach is that is the iso surface analysis, which actually study the topology and dynamics of the iso level surface.

In premixed flame, this iso surface is called progress variable and the non premixed case is the iso mixture fraction, and the second approach is flame normal analysis there you gather the information in the direction normal to the flame surface and do the analysis or you can have some point analysis which collect information at every point and do the analysis or each frame analysis. Now flamelet model or PDF models are respectively a based on frame normally analysis and one point.

So when you look at the flame normal analysis, that means you try to derive your system or convert the system along the flame normal directions. So that is where you get flamelet kind of model that means you try to define your turbulent flame front to be ensemble of small laminate flame brush or when you try to collect based on point analysis. This is where you get the PDF kind of approach which we have seen in the turbulent case.

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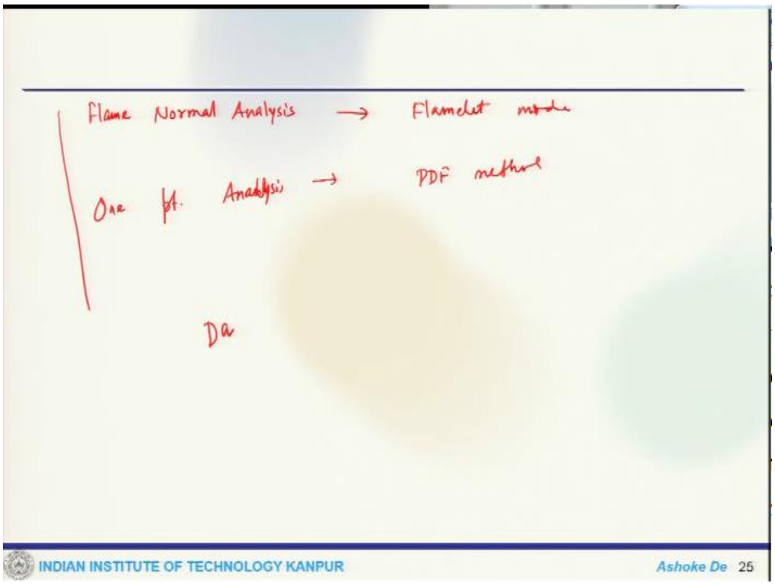

Flame Normal Analysis → Flamelet mode

One pt. Analysis → PDF method

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Now, that means if you have claimed normal analysis. That will lead to flamelet model so which means the structure normal to the flame surface in turbulent flame is assumed to be the same as the laminar flame. So, probability density function of the independent variable CRJD is used or if you use one-point analysis.

That will lead to PDF kind of methods. Further the equation of probability density function fluctuation at one point are modeled and solved. Now the success accuracy of these kind of models depend on the type of flame so there is premixed, non premixed, partially premixed but one important things which will come into the picture is the Damkohler number which is the ratio of 2-time scale between air flow and kinetics.

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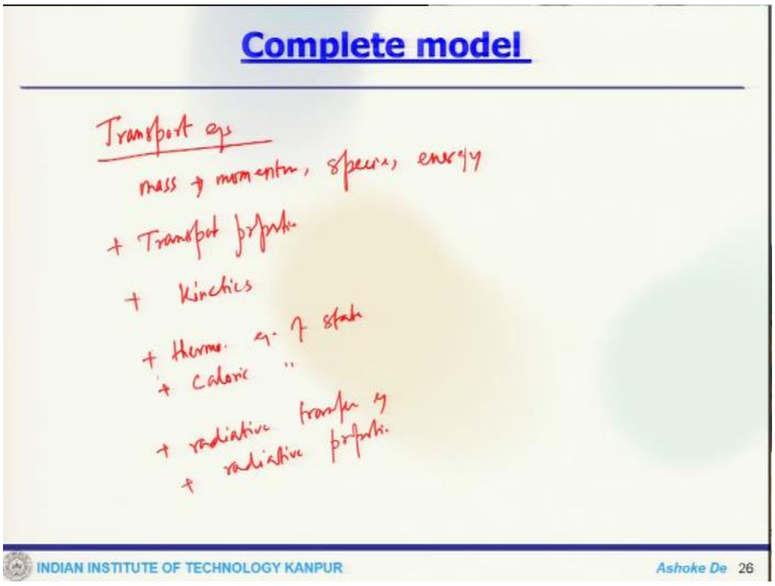

Complete model

Transport eqs

mass + momentum, species, energy

+ Transport propts.

+ Kinetics

+ thermo. eq. of state

+ caloric "

+ radiative transfer eq

+ radiative propts.

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So complete the model we have transport equation which is mass, momentum, species, energy or temperature plus transport properties, kinetics and other things like thermodynamics equation of state, caloric equation of state, radiative transfer equation, radiative properties etcetera.

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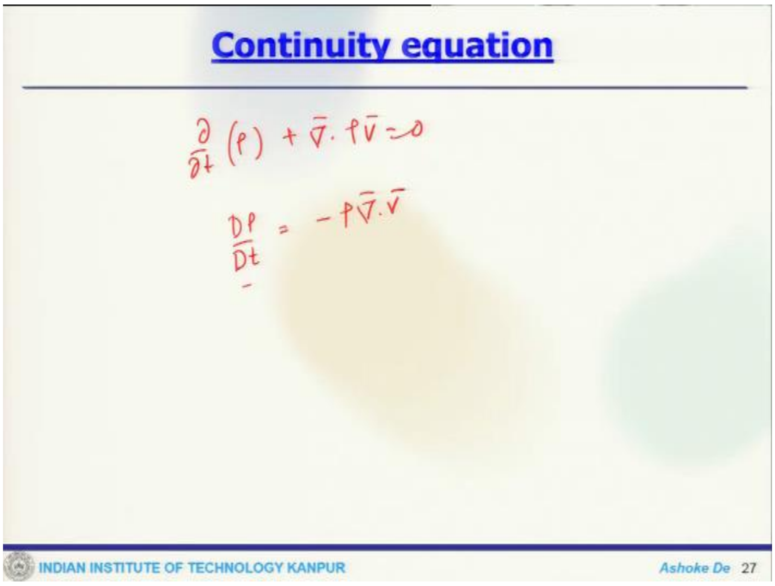

Continuity equation

$$\frac{\partial}{\partial t}(\rho) + \bar{\nabla}\cdot\rho\bar{v} = 0$$

$$\frac{D\rho}{Dt} = -\rho\bar{\nabla}\cdot\bar{v}$$

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So we can start with the continuity equation and that is one can write

$$\frac{\partial(\rho)}{\partial t} + \bar{\nabla}.\rho\bar{v} = 0$$

which will get us

$$\frac{D\rho}{Dt} = -\rho\bar{\nabla}\,\bar{v}$$

Because this is reacting system due to temperature the variation of density is there, so one has to solve this variable density situation.

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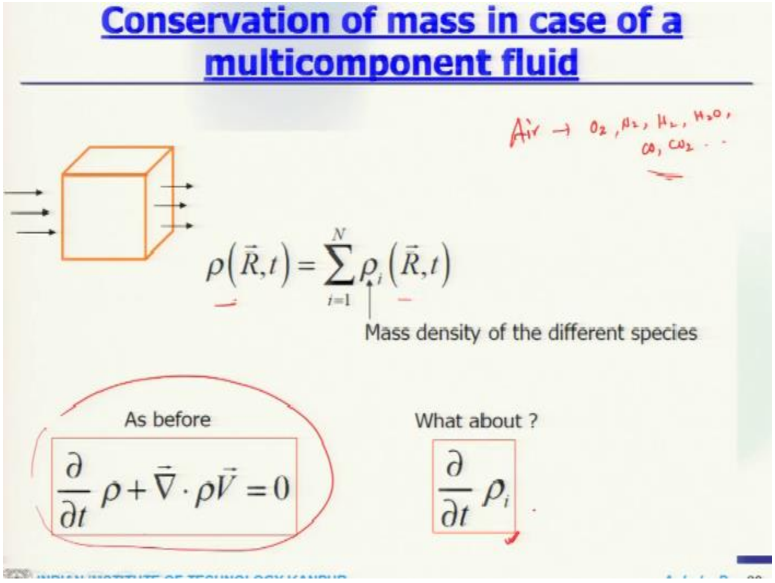

Conservation of mass in case of a multicomponent fluid

Air → O_2, N_2, H_2, H_2O, CO, CO_2 . . .

$$\rho(\vec{R},t) = \sum_{i=1}^{N} \rho_i(\vec{R},t)$$

Mass density of the different species

As before

$$\boxed{\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\rho\vec{V} = 0}$$

What about ?

$$\boxed{\frac{\partial}{\partial t}\rho_i}$$

Now, if you have multi-component fluid which typically happens or present in the system, you need to get the system density to be some of these different species. For example, if you consider air. Air has by and large oxygen, nitrogen, but then you can have H_2 some amount of H_2O some amount of CO, CO_2 and so on. But this may be by volume very less but there are multiple species, when you have multiple species the summation of that density would give you the total density.

So like we can have the system density it will satisfy the continuity equation. But what about these term? Now at the total density or the mixture density that satisfies the continuity what happens to individual term? Will see how this leads to our individual species mass transfer equation.

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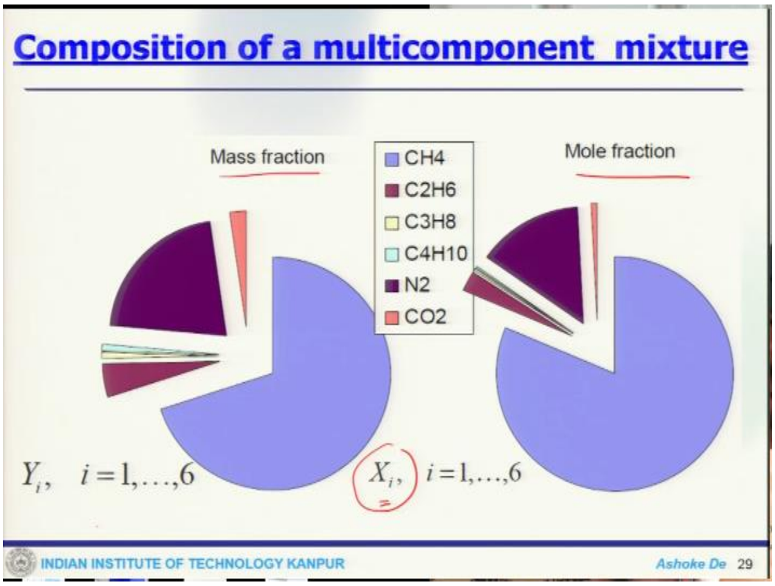

Composition of a multicomponent mixture

$Y_i, \quad i = 1,\ldots,6$

$X_i, \quad i = 1,\ldots,6$

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Now, as I said that you can have the multiple species in a system and then they could have different proportion one where to represent that by mass fraction, and other option is the mole fraction that we have seen and typically we use this is the representation for the mole fraction and this would be for the mass fraction.

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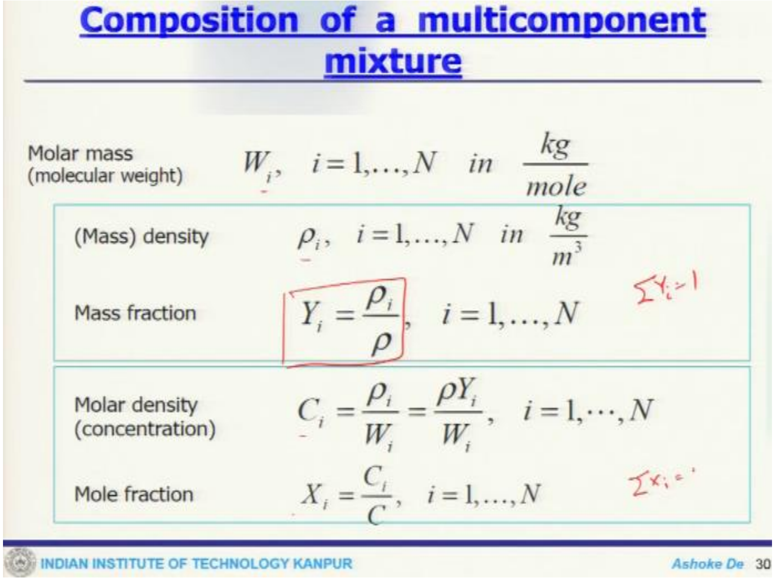

Composition of a multicomponent mixture

Molar mass (molecular weight) $W_i, \quad i = 1, \ldots, N \quad in \quad \frac{kg}{mole}$

(Mass) density $\rho_i, \quad i = 1, \ldots, N \quad in \quad \frac{kg}{m^3}$

Mass fraction $\boxed{Y_i = \frac{\rho_i}{\rho}}, \quad i = 1, \ldots, N$ $\quad \sum Y_i = 1$

Molar density (concentration) $C_i = \frac{\rho_i}{W_i} = \frac{\rho Y_i}{W_i}, \quad i = 1, \cdots, N$

Mole fraction $X_i = \frac{C_i}{C}, \quad i = 1, \ldots, N$ $\quad \sum X_i = 1$

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So, just to recap these things. You have molar mass W_i then mass density and mass fraction would be $\frac{\rho_i}{\rho}$. This is how and the total mass of the system should be 1 similarly molar density. You have a mole fraction and summation of mole fraction also should be 1.

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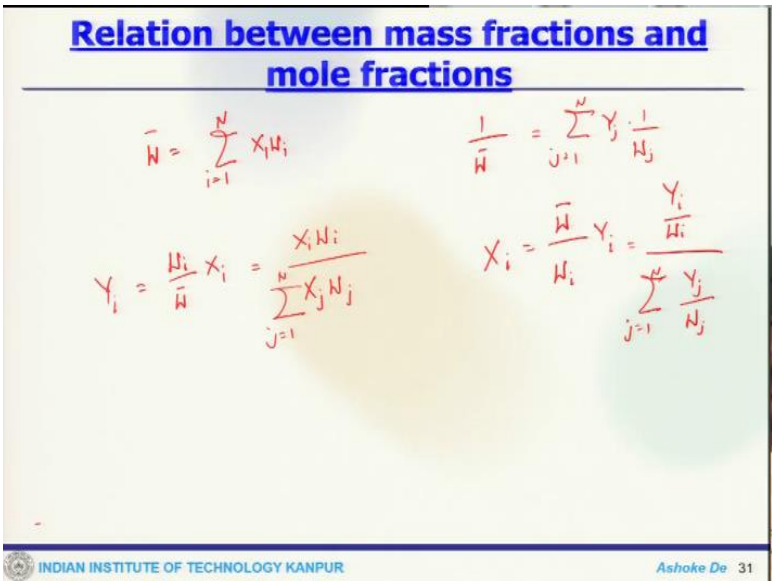

Relation between mass fractions and mole fractions

$$\bar{W} = \sum_{i=1}^{N} X_i W_i \qquad \frac{1}{\bar{W}} = \sum_{j=1}^{N} Y_j \cdot \frac{1}{W_j}$$

$$Y_i = \frac{W_i}{\bar{W}} X_i = \frac{X_i W_i}{\sum_{j=1}^{N} X_j W_j} \qquad X_i = \frac{\bar{W}}{W_i} Y_i = \frac{\frac{Y_i}{W_i}}{\sum_{j=1}^{N} \frac{Y_j}{W_j}}$$

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Now you can have mean molar mass W, which is

$$\bar{W} = \sum_{i=1}^{N} X_i W_i$$

then

$$\frac{1}{\bar{W}} = \sum_{j=1}^{N} Y_j \frac{1}{W_j}$$

So we can have conversion from one to the other Y_i equals to

$$Y_i = \frac{W_i}{\bar{W}} X_i = \frac{X_i W_i}{\sum_{i=1}^{N} X_j W_j}$$

and X_i is

$$X_i = \frac{\bar{W}}{W_i} Y_i = \frac{\frac{Y_i}{W_i}}{\sum_{j=1}^{N} \frac{Y_j}{N_j}}$$

So one can represent sometimes the mass fraction and sometime that.

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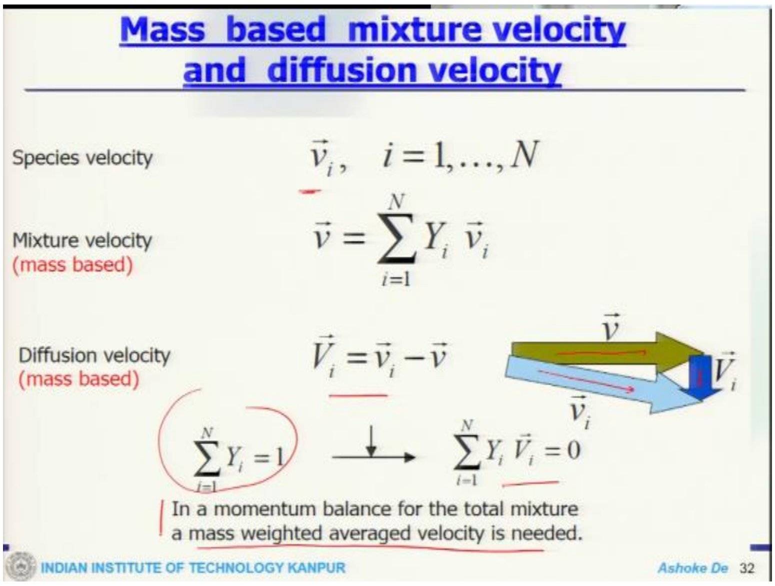

Mass based mixture velocity and diffusion velocity

Species velocity $\vec{v}_i, \quad i = 1, \ldots, N$

Mixture velocity (mass based) $\vec{v} = \sum_{i=1}^{N} Y_i \vec{v}_i$

Diffusion velocity (mass based) $\vec{V}_i = \vec{v}_i - \vec{v}$

$$\sum_{i=1}^{N} Y_i = 1 \longrightarrow \sum_{i=1}^{N} Y_i \vec{V}_i = 0$$

In a momentum balance for the total mixture a mass weighted averaged velocity is needed.

So this is another important thing that mass base mixture velocity and the diffusion velocity. So the species velocity is V^i which is acting in this direction and the mixture velocity which is summation of Y_i and V_i which will be acting on this. So the diffusion velocity is the difference between these 2 velocities.

So the species which are, they are in the system that summation Y_i is 1 and if we take the product of Y_i by V_i that should be 0, so that means in a momentum balance for the total mixture a mass weighted average velocity is needed. This is an important point to be noted here that mass weighted.

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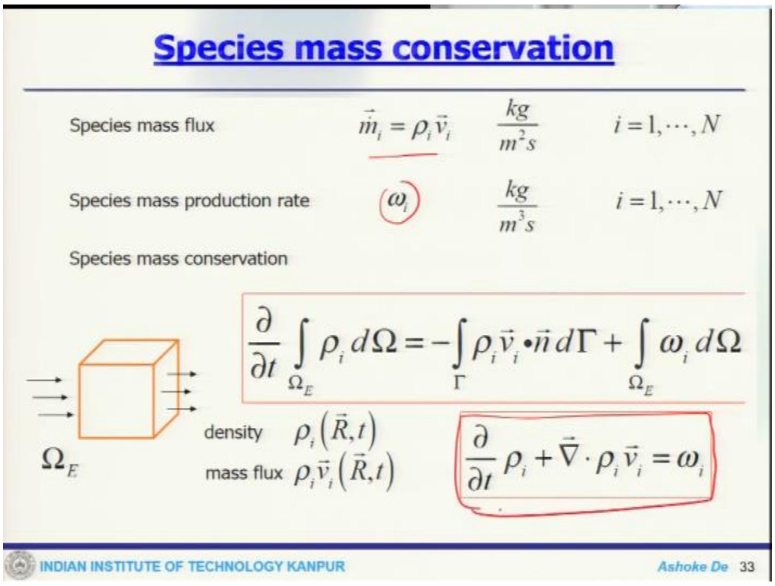

Species mass conservation

Species mass flux $\vec{m}_i = \rho_i \vec{v}_i$ $\frac{kg}{m^2 s}$ $i = 1, \cdots, N$

Species mass production rate ω_i $\frac{kg}{m^3 s}$ $i = 1, \cdots, N$

Species mass conservation

$$\frac{\partial}{\partial t}\int_{\Omega_E} \rho_i \, d\Omega = -\int_{\Gamma} \rho_i \vec{v}_i \bullet \vec{n} \, d\Gamma + \int_{\Omega_E} \omega_i \, d\Omega$$

density $\rho_i(\vec{R}, t)$

mass flux $\rho_i \vec{v}_i(\vec{R}, t)$

$$\boxed{\frac{\partial}{\partial t}\rho_i + \vec{\nabla} \cdot \rho_i \vec{v}_i = \omega_i}$$

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Now, we have species mass flux, which is $\rho_i v_i$ then they also due to the reaction there would be species production rate or destruction rate. So that is ω_i then for this small control volume one can get the species mass conservation. So which in term get you $\frac{\partial \rho_i}{\partial t}$. So this is your species mass conservation equation and individual.

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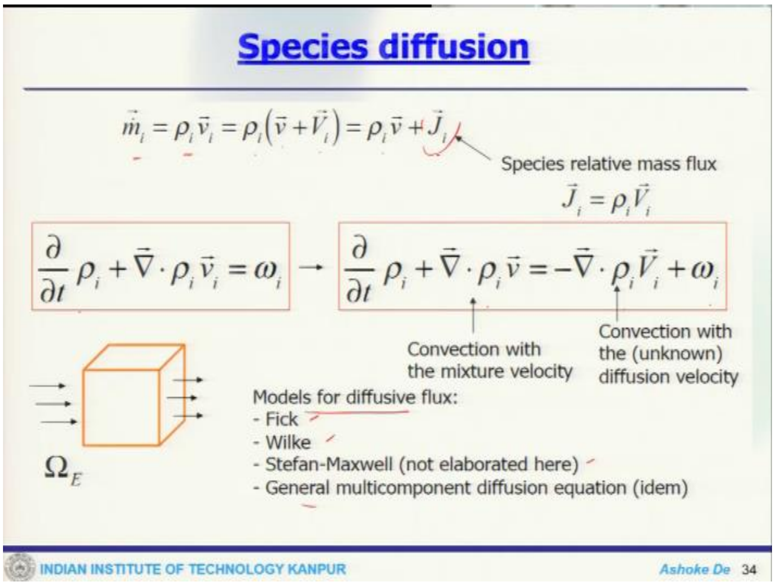

Species diffusion

$$\vec{m}_i = \rho_i \vec{v}_i = \rho_i(\vec{v} + \vec{V}_i) = \rho_i \vec{v} + \vec{J}_i$$

Species relative mass flux

$$\vec{J}_i = \rho_i \vec{V}_i$$

$$\frac{\partial}{\partial t}\rho_i + \vec{\nabla} \cdot \rho_i \vec{v}_i = \omega_i \rightarrow \frac{\partial}{\partial t}\rho_i + \vec{\nabla} \cdot \rho_i \vec{v} = -\vec{\nabla} \cdot \rho_i \vec{V}_i + \omega_i$$

Convection with the mixture velocity

Convection with the (unknown) diffusion velocity

Models for diffusive flux:
- Fick
- Wilke
- Stefan-Maxwell (not elaborated here)
- General multicomponent diffusion equation (idem)

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So if I expand this term of the mass flux, this is

$$\overrightarrow{\dot{m}_i} = \rho_i \overrightarrow{v_i} = \rho_i(\bar{v} + \overline{V_i}) = \rho_i \bar{v} + \overline{J_i}$$

So if I put these things here in the equation of the species mass conservation and what we get that this is convection with the diffusion velocity and this is now this particular term there are different models for this diffusion flux.

There is Fick's model, Wilke's model, Stefan-Maxwell model, General multi component diffusion. So there are different ways one can represent this models for this.

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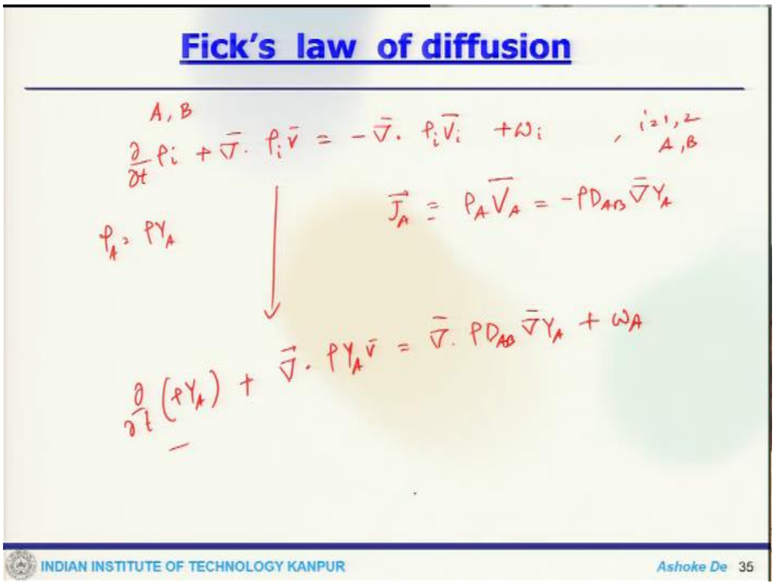

Fick's law of diffusion

A, B

$$\frac{\partial}{\partial t}\rho_i + \bar{\nabla}\cdot\rho_i\bar{v} = -\bar{\nabla}\cdot\rho_i\bar{V_i} + \omega_i \quad , \quad \begin{matrix} i=1,2 \\ A,B \end{matrix}$$

$$\rho_A = \rho Y_A$$

$$\vec{J_A} = \rho_A\overline{V_A} = -\rho D_{AB}\bar{\nabla}Y_A$$

$$\downarrow$$

$$\frac{\partial}{\partial t}(\rho Y_A) + \vec{\nabla}\cdot\rho Y_A\bar{v} = \bar{\nabla}\cdot\rho D_{AB}\bar{\nabla}Y_A + \omega_A$$

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Now that is why if you use Fick's law of diffusion. So if you take a case of binary system with 2 species A and B, then

$$\frac{\partial\rho_i}{\partial t} + \overline{\nabla}.\rho_i\bar{v} = -\overline{\nabla}.\rho_i\overline{v_i} + \omega_i$$

here i equals to 1 and 2 which is rather A and B. So ρ_A would be ρY_A. So that means

$$\overrightarrow{J_A} = \rho_A\overline{V_A}$$

and from here what we get

$$\frac{\partial(\rho Y_A)}{\partial t} + \overline{\nabla}.\rho Y_A\bar{v} = \overline{\nabla}.\rho_i D_{AB}\overline{\nabla}.Y_A + \omega_A$$

So this is a mass fraction equation for species provided density mixture velocity diffusion constant all these are known.

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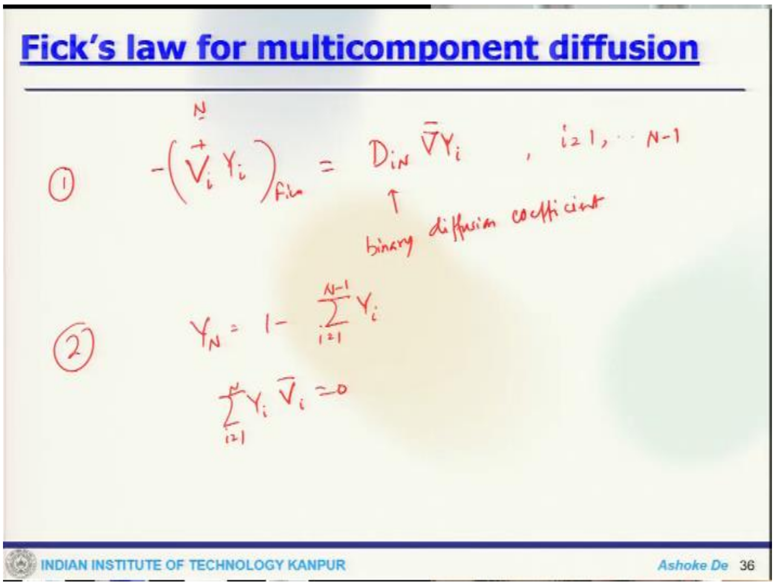

Fick's law for multicomponent diffusion

① $-\left(\vec{V}_i Y_i\right)_{Fick} = \overset{N}{D_{iN}} \bar{\nabla} Y_i \quad , \quad i=1, \cdots N-1$

↑ binary diffusion coefficient

② $Y_N = 1 - \sum_{i=1}^{N-1} Y_i$

$\sum_{i=1}^{N} Y_i \vec{V}_i = 0$

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Now we can use the Fick's law for multi-component diffusion, so we can select one carrier gas. For example, let us say we take nitrogen then you solve the species transport equation with diffusion velocity equals to $D_{iN}\overline{\nabla}\, Y_i$ where i equals to 1 to N - 1 and this is nothing but binary diffusion coefficient. So then we can solve for the carrier species that is number 1. Step 2 we can solve for the carrier species which is

$$Y_N = 1 - \sum_{i=1}^{N-1} Y_i$$

so which guarantees that summation of $Y_i\, \overline{V_i}$ is 0.

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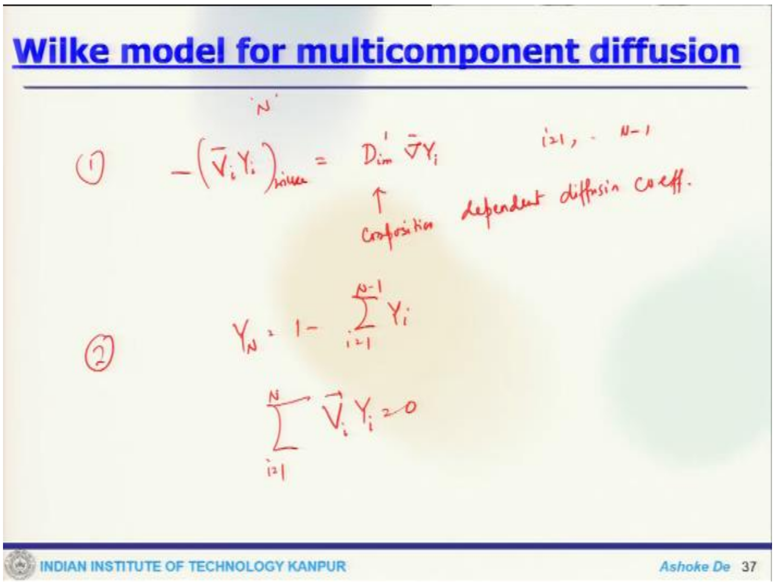

Wilke model for multicomponent diffusion

① $-\left(\bar{V}_i Y_i\right)_{Wilke} = \overset{'N'}{D'_{im}} \bar{\nabla} Y_i \qquad i=1, \cdot\ N-1$

↑ Composition dependent diffusion coeff.

② $Y_N = 1 - \sum_{i=1}^{N-1} Y_i$

$\sum_{i=1}^{N} \vec{V}_i Y_i = 0$

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So that is how similarly? We can use the Wilke's model for multicomponent diffusion where again we have to select a carrier gas, let us say nitrogen then step one, we solved for the transport equation with Wilke D_{iN} bar where i equals to 1 to N -1, here this guy is the composition dependent diffusion coefficient. Secondly we solve for the carrier species, which is 1 minus summation of Y_i and that guarantees Y_i equals to 0 for i goes to 1 to N.

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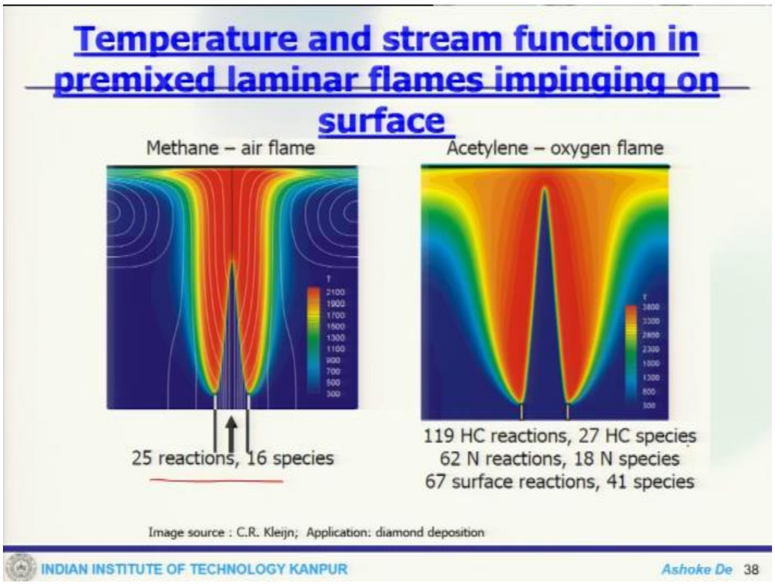

Temperature and stream function in premixed laminar flames impinging on surface

Methane – air flame

Acetylene – oxygen flame

25 reactions, 16 species

119 HC reactions, 27 HC species
62 N reactions, 18 N species
67 surface reactions, 41 species

Image source : C.R. Kleijn; Application: diamond deposition

So we can see some example where the temperature and the stream function in a premixed laminar flame impinging on a surface. This is a methane air flame which 25 reactions 16 species. This is acetylene-oxygen flame with so many reactions.

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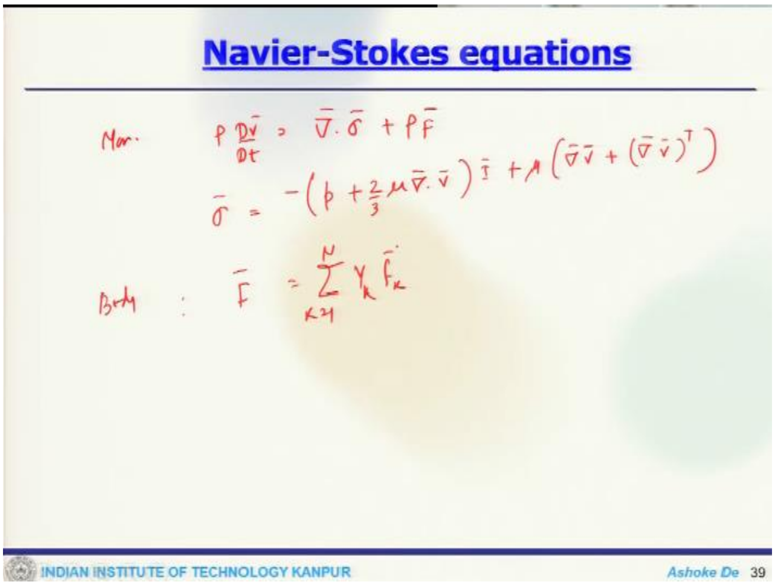

Navier-Stokes equations

Mom. $\rho \frac{D\bar{v}}{Dt} = \bar{\nabla}\cdot\bar{\sigma} + \rho\bar{F}$

$\bar{\sigma} = -\left(p + \frac{2}{3}\mu\bar{\nabla}\cdot\bar{v}\right)\bar{I} + \mu\left(\bar{\nabla}\bar{v} + (\bar{\nabla}\bar{v})^T\right)$

Body : $\bar{F} = \sum_{k=1}^{N} Y_k \bar{f}_k$

So depending on the situation the flame, a shape and all these things changes, now momentum transport you get

$$\rho\frac{D\bar{v}}{Dt} = \bar{\nabla}.\bar{\sigma} + \rho\,\bar{F}$$

where σ is the stress tensor, which is

$$\sigma = -\left(p + \frac{2}{3}\mu\bar{\nabla}.\bar{v}\right)\bar{J} + \lambda(\bar{\nabla}.\bar{v} + (\bar{\nabla}.\bar{v})^T$$

Now body forces is

$$\bar{F} = \sum_{k=1}^{N} Y_K\overline{F_k}$$

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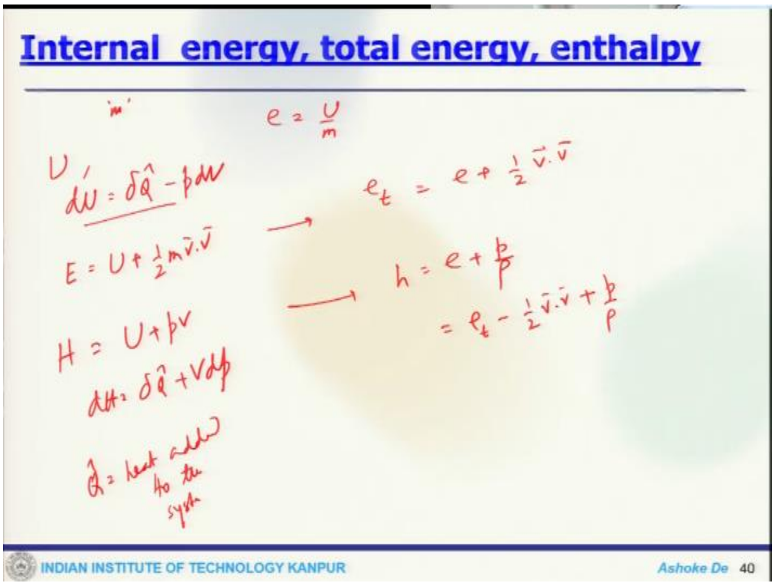

Internal energy, total energy, enthalpy

'm'

$e = \frac{U}{m}$

$U,$

$\underline{dU = \delta\hat{Q} - p\,dV}$

$E = U + \frac{1}{2}m\bar{v}.\bar{v}$

$\longrightarrow \quad e_t = e + \frac{1}{2}\bar{v}.\bar{v}$

$H = U + pV$

$dH = \delta\hat{Q} + V\,dp$

$\longrightarrow \quad h = e + \frac{p}{\rho}$

$= e_t - \frac{1}{2}\bar{v}.\bar{v} + \frac{p}{\rho}$

$\hat{Q}$ = heat added to the system

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Now we can have some internal energy, total energy and enthalpy for let us say we consider mass m then specific internal energy e would be U by m where internal energy U can be used as du equals to del Q minus P dv which you get from the first law of thermodynamics and this is U plus half m and total enthalpy is U plus PV where dH equals to del Q plus Vdp, here Q is the heat added to the system.

So this is the per unit mass. So specific total energy per unit mass would be e plus half V. Specific enthalpy would be e plus P by rho or e t minus half P by rho. So these are some of the terminology which will be required.

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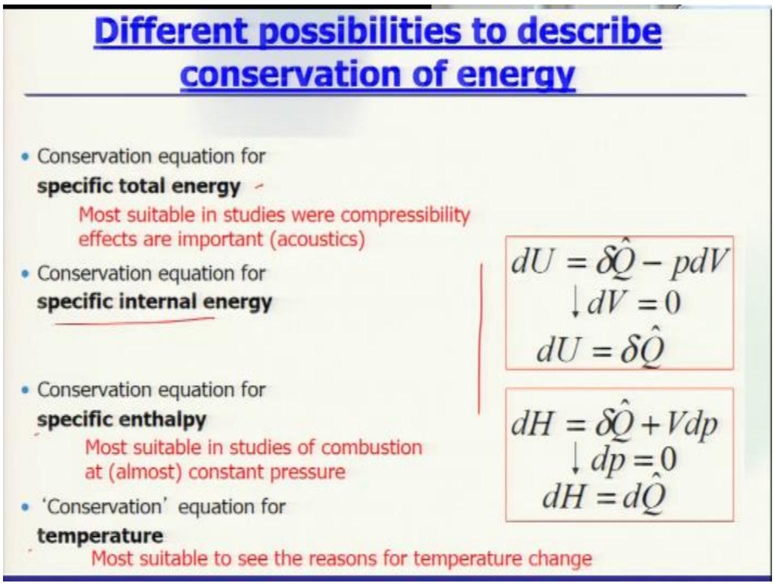

Different possibilities to describe conservation of energy

- Conservation equation for **specific total energy**
  Most suitable in studies were compressibility effects are important (acoustics)
- Conservation equation for **specific internal energy**
- Conservation equation for **specific enthalpy**
  Most suitable in studies of combustion at (almost) constant pressure
- 'Conservation' equation for **temperature**
  Most suitable to see the reasons for temperature change

$$dU = \delta\hat{Q} - pdV \quad \downarrow dV = 0 \quad dU = \delta\hat{Q}$$

$$dH = \delta\hat{Q} + Vdp \quad \downarrow dp = 0 \quad dH = d\hat{Q}$$

Now different possibilities to describe the conservation of energy, so the either one can do that in terms of specific total energy, which is more suitable in studies where compressibility effects are important or specific internal energy or specific enthalpy this is also study. I mean the specific enthalpy is quite often used or more suitable for this kind of combustion process or the temperature.

These are suitably used in incompressible situation where the density variation is not there due to change. This is what already we have talked about from the connectivity between internal energy and enthalpy analytics.

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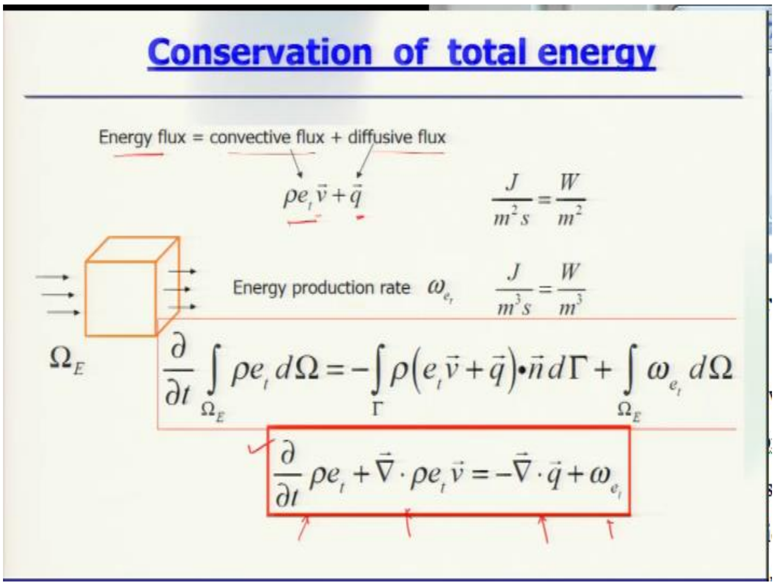

Conservation of total energy

Energy flux = convective flux + diffusive flux

$$\rho e_t \vec{v} + \vec{q} \qquad \frac{J}{m^2 s} = \frac{W}{m^2}$$

Energy production rate ω_{e_t} $\quad \frac{J}{m^3 s} = \frac{W}{m^3}$

$$\frac{\partial}{\partial t}\int_{\Omega_E} \rho e_t \, d\Omega = -\int_{\Gamma} \rho\left(e_t \vec{v} + \vec{q}\right)\cdot\vec{n}\, d\Gamma + \int_{\Omega_E} \omega_{e_t}\, d\Omega$$

$$\boxed{\frac{\partial}{\partial t}\rho e_t + \vec{\nabla}\cdot\rho e_t \vec{v} = -\vec{\nabla}\cdot\vec{q} + \omega_{e_t}}$$

So now if you look at the conservation of the total energy, so the energy flux there will be 2 components one is the convective flux another is the diffusive flux. So this is the component coming from the convective flux and this is the component due to diffusive flux. So if we write down in terms of the volume integral, this is what we get there is an unsteady term convection diffusion and source term of the energy.

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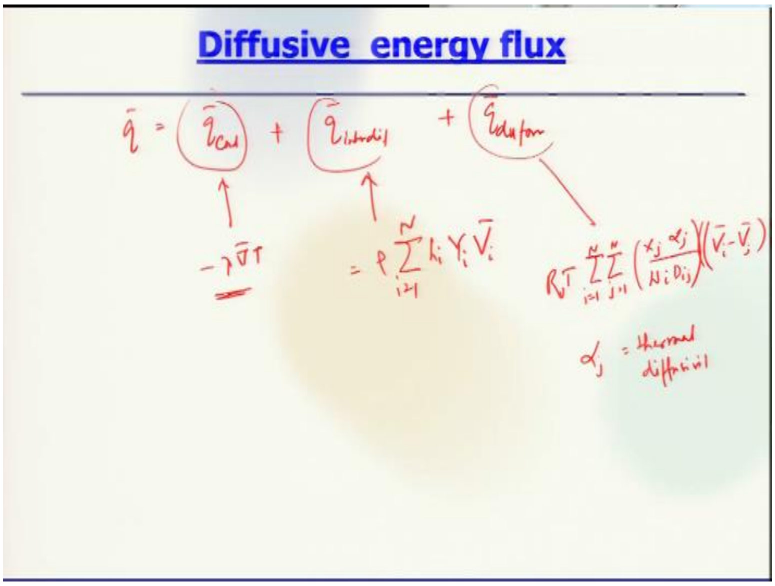

Diffusive energy flux

$$\bar{q} = \bar{q}_{cond} + \bar{q}_{interdiff} + \bar{q}_{dufour}$$

$$-\lambda \bar{\nabla} T$$

$$= \rho \sum_{i=1}^{N} h_i Y_i \bar{V}_i$$

$$R_u T \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\frac{X_j \alpha_j}{W_i D_{ij}}\right)(\bar{V}_i - \bar{V}_j)$$

α_j = thermal diffusivity

So we can see the individual term like this q you can have q convection you can have inter diffusion or you can have effect of dufour. So we use the fourier law of heat convection where this can be represented as lambda del T. This is represented as rho summation of i equals to 1 to N h i Y i V i and the dufour effect is defined as R u T summation of i equals to 1 to N summation of j equals to 1 to N X j alpha j W i D i j V i minus V j where alpha j is thermal diffusivity.

So this contribute convection contribute due to the thermal gradient inter diffusion is due to the species diffusion and the dufour effect. This is the heat flux due to gradient in species concentration. So this is a counterpart of (()) (25:53) effect, which is also mostly negligible. This is flux due to pressure gradient.

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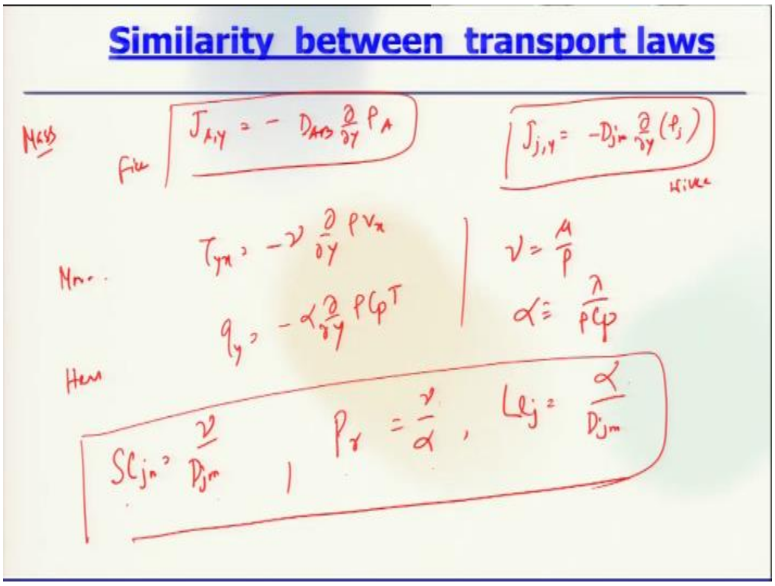

Similarity between transport laws

Mass

Fick $J_{A,y} = -D_{AB}\frac{\partial}{\partial y}\rho_A$

$J_{j,y} = -D_{jm}\frac{\partial}{\partial y}(\rho_j)$

Wilke

Mom..

$\tau_{yx} = -\nu\frac{\partial}{\partial y}\rho v_x$

$\nu = \frac{\mu}{\rho}$

$q_y = -\alpha\frac{\partial}{\partial y}\rho C_p T$

$\alpha = \frac{\lambda}{\rho C_p}$

Heat

$Sc_{jm} = \frac{\nu}{D_{jm}}$, $Pr = \frac{\nu}{\alpha}$, $Le_j = \frac{\alpha}{D_{jm}}$

Now we can see the similarity between transport laws. So we have mass where J is minus D AB rho A which is from Fick's law then J j, y is minus D jm by del del y of rho j. This is what we got from Wilke's, momentum, which is mass diffusion, momentum we have tau yx equal to nu del del y by rho v x heat, a fourier where q y equals to minus alpha del del y of rho C p T. So nu is mu by rho, alpha is lambda by rho C P. So, the some dimension less parameter, which are quite important.

Is that Schmidt number is nu by D jm then Prandtl number, which is nu by alpha and Lewis number which is alpha by D jm .So these are the non dimensional parameter, which so there is a similarity or rather the connectivity between different law. So the Schmidt number which connects mass diffusion to the momentum. Prandtl number is a mass diffusion to or a momentum to thermal, Lewis number mass to thermal.

So these are the non dimensional parameter then one need to know, so we will stop here today and continue this discussion in the subsequent lecture.